11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

MC Simulation of THz Quantum Cascade Lasers

C. Jirauschek, M. Manenti*, G. Scarpa, and P. Lugli
Institute for Nanoelectronics, TU München, Arcisstraße 21, 80333 München, Germany
*Dept. Electronic Engineering, Università Roma "Tor Vergata", Italy
e-mail: jirauschek@mytum.de

INTRODUCTION

In the following, we show simulation results for two types of THz quantum cascade lasers (QCLs), GaAs-based QCLs and Si/SiGe QCLs, which have enormous potential as compact and efficient THz sources.

Our simulator includes the following feature: Solution of the coupled Schrödinger-Poisson equation to determine the band diagram and the subband energies and wavefunctions; simulation of electron dynamics including all essential scattering mechanisms (electron-electron, electron-LO phonon, electron-acoustic phonon); coupling of the Schrödinger-Poisson solver to the MC simulation; calculation of gain spectra; determination of the subband electronic temperature.

GAAS/ALGAAS THZ QCL

We report on Monte Carlo (MC) simulations aimed at the design and optimization of GaAs-based THz quantum cascade lasers operating between 2 and 4 THz, and at the modeling of their operation. We have focused our analysis on a series of QCL structures operating in the range of 3.2 – 3.8 THz reported in Refs. [1]-[3]. The results have been positively compared with experimental results [4]. Positive gain has been demonstrated in the simulation, and indeed lasing has been achieved on these reported fabricated structures. The electron temperatures agree well with the experimental ones [4].

The MC simulation allows the identification of the processes responsible for the non ideal laser performance (high threshold currents and low operation temperatures). Figure 1 shows the band diagram and subband wavefunctions for the laser structure operating at 3.2 THz, the calculated gain spectrum at two different temperatures is shown in Figure 2.

SI/SIGE THZ QCL

THz QCLs based on Si/SiGe have the potential to operate at room temperature due to the absence of polar phonon scattering. However, no lasing in such structures has been observed up to date. Simulations are necessary to identify the reasons and help develop a working design. In order to simulate the hole-based Si/SiGe QCLs, we have modified the MC program described above to account for both light and heavy hole bands and for the proper phonon scattering active in silicon-based materials. We still use an envelope function description of the subbands, fitting the effective mass to those obtained from a k.p calculation. Improvements of the method will be presented at the conference. We have simulated a QCL structure which is also based on the phonon depopulation principle of the GaAs laser discussed above. Figure 3 shows the band diagram and subband wavefunctions of a Si/SiGe QCL, and Figure 4 displays the corresponding hole distribution functions for a lattice temperature of 150 K. The corresponding effective temperatures range from 185 K to 220 K.

CONCLUSION

In conclusion, we have shown that the Monte Carlo simulation allows an effective design of QCLs for THz applications. Improvement of the model to include a k.p description of the hole subbands for the p-type structures will be presented at the conference.

REFERENCES

[1] B. S. Williams, S. Kumar, H. Callebaut, Q. Hu and J.L.Reno, *Terahertz quantum-cascade laser operating up to 137 K*, Appl. Phys. Lett. **83**, 5142 (2003).

[2] B. S. Williams, S. Kumar, H. Callebaut, Q. Hu and J.L.Reno, *3.4-THz quantum cascade laser based on longitudinal-optical-phonon scattering for depopulation*, Appl. Phys. Lett. **82**, 1015 (2003).

[3] S. Kumar, B. S. Williams, S. Kohen, Q. Hu and J. L.Reno, *Continuous-wave operation of terahertz quantum-cascade*

lasers above liquid-nitrogen temperature, Appl. Phys. Lett. **84**, 2494 (2004).

[4] M. S. Vitiello, G. Scamarcio, V. Spagnolo, B. S. Williams, S. Kumar, Q. Hu and J. L. Reno, *Measurement of subband electronic temperatures and population inversion in THz quantum-cascade lasers*, Appl. Phys. Lett. **86**, 111115 (2005).

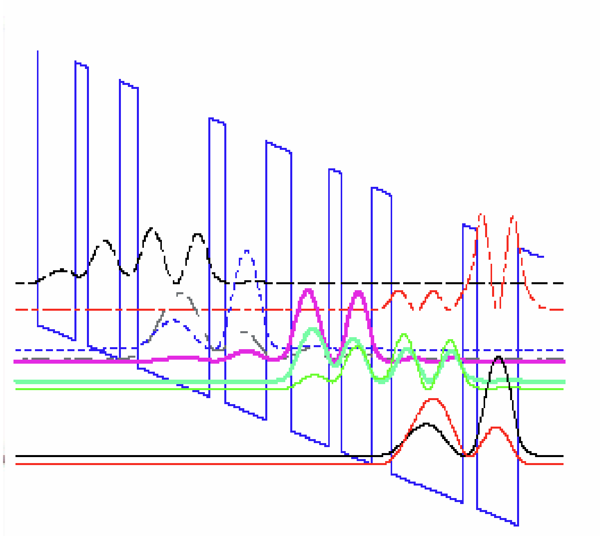

Fig. 1: Band diagram and subband wavefunctions of GaAs-based QCL.

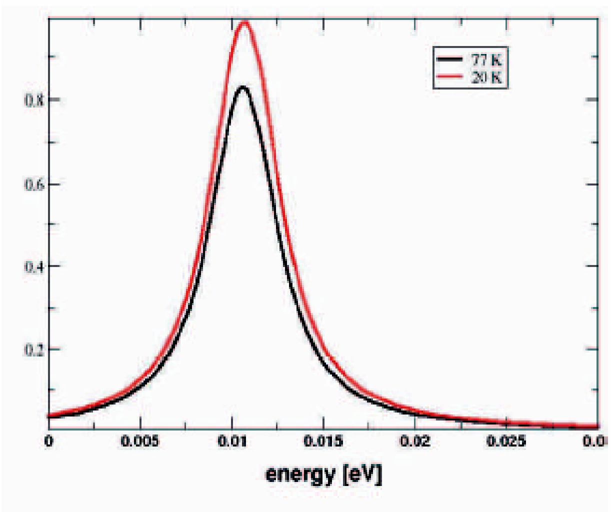

Fig. 2: Calculated gain spectrum for a lattice temperature of 20 K (red) and 77 K (black).

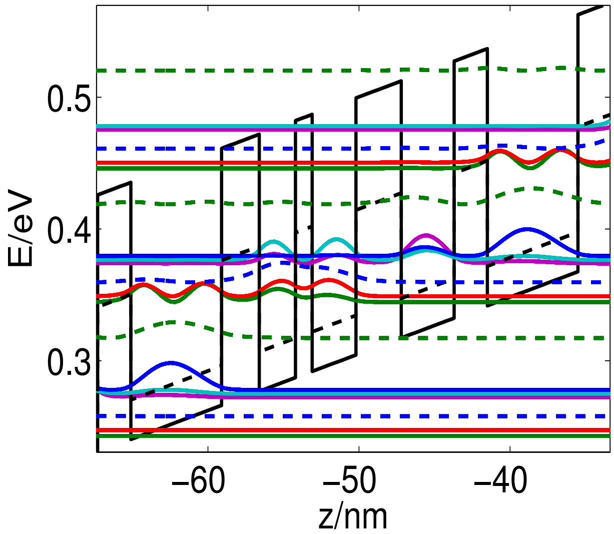

Fig. 3: Band diagram and subband wavefunctions of Si/SiGe QCL for light hole (dashed lines) and heavy holes (solid lines) band.

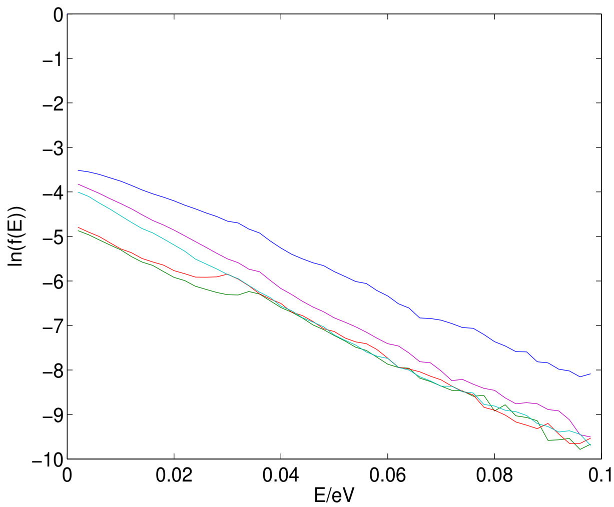

Fig. 4: Heavy hole distribution functions for a lattice temperature of 150 K for the levels shown in Fig. 4 (same color coding).